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Structure of the stereoisomers of tetrasubstituted p--butylcalix[4]arene containing a morpholine fragment: Data of 1D and 2D (NOESY) NMR spectroscopy

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Abstract

The structure of three isomers of 5,11,17,23-tetra-t-butyl-25,26,27,28-tetrakis[(morpholidocarbonyl) methoxy]-2,8,14,20-tetrathiacalix[4]arene in conformations of partial cone, 1,3-alternant and cone was studied by the methods of 1D and 2D (NOESY) 1H and 13C NMR spectroscopy in conjunction with computational modeling (semiempirical quantum-chemical PM3 calculations). Characteristic cross-peaks for each conformer in the two-dimensional NOESY spectra were established. It is found that unsymmetrical conformation of partial cone is more "flattened" as compared with highly symmetrical 1,3-alternant and cone conformations, while OCH 2C(O)NC4H8O substituent is located in the exo-position. Theoretical modeling is found to be more consistent with the experimental data for highly symmetrical conformations. © 2009 Pleiades Publishing, Ltd.

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